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Consistent thermodynamic properties of lipids systems

Larissa P.Cunico^a, Roberta Ceriani^b, Bent Sarup^c, Jeong W. Kang^d,

John P. O'Connell^e, Rafiqul Gani^a

^a Computer Aided Process-Product Engineering Center (CAPEC), Department of Chemical and Biochemical Engineering, Technical University of Denmark, DK-2800, Kgs. Lyngby, Denmark.

^b Faculty of Chemical Engineering, State University of Campinas, Av. Albert Einstein 500, Cidade Universitária Zeferino Vaz, 13083-852 Campinas-SP, Brazil. ^cVegetable Oil Technology Business Unit, Alfa Laval Copenhagen A/S, Maskinvej 5, DK-2860 Soeborg, Denmark. ^dDepartment of Chemical and Biological Engineering, Korea University, 5-1 Anam-Dong, Sungbuk-Ku, Seoul 136-701, South Korea. ^e Department of Chemical Engineering, University of Virginia, Charlottesville, VA 22901, USA.

*Corresponding author: E-mail address: rag@kt.dtu.dk (R. Gani); Phone no: +45-45252882; Fax no: +45-45932906.

Physical and thermodynamic properties of pure components and their mixtures are the basic requirement for process design, simulation, and optimization. In the case of lipids, our previous works[1-3] have indicated a lack of experimental data for pure components and also for their mixtures. To contribute in this area, experimental data were obtained using the Differential Scanning Calorimetry (DSC) technique for isobaric vapor-liquid equilibrium (VLE) of two binary mixtures at two different pressures (1.2 and 2.5 KPa): system 1 [monoacylglycerol (monocaprylin) + fatty acid (palmitic acid)] and system 2 [monoacylglycerol (monocaprylin) + fatty ester (methyl stearate)]. System 1 is relevant in the purification steps of the deodorizer distillates while system 2 is relevant in the purification steps of biodiesel and bioglycerin. A non-ideal behavior is revealed for both systems at the two different pressures, with azeotrope behavior observed. Available thermodynamic consistency tests for TPx data were applied before performing parameter regressions for Wilson, NRTL, UNIQUAC and original UNIFAC models. The relevance of enlarging experimental databank of lipids systems data in order to improve the performance of predictive thermodynamic models was confirmed in this work by analyzing the calculated values of original UNIFAC model. For solid-liquid equilibrium (SLE) data, new consistency tests have been developed [2]. Some of the developed tests were based in the quality tests proposed for VLE data by Kang et al. [4] and a methodology that combines solute activity coefficients in the liquid phase at infinite dilution and a theoretically based term to account for the non-ideality in dilute solutions are discussed. In this work, case studies considering the methodology proposed for SLE thermodynamic consistency tests and data from open literature and databases such as NIST-TDE®, DIPPR® and DECHEMA® are presented. The SLE consistency test and data evaluation is performed in a software containing option for data analysis, model analysis and parameter regression.

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